



# **Modeling and Simulation of Plasma-Assisted Ignition and Combustion**

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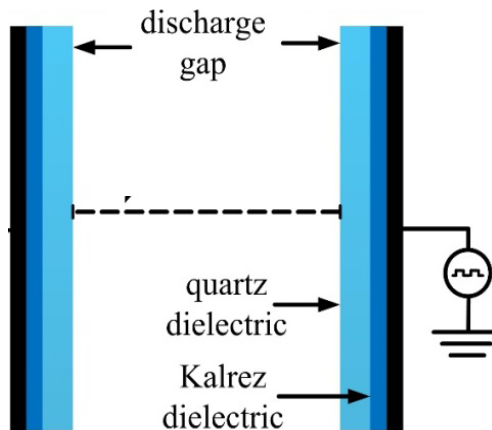


*AFOSR MURI “Fundamental Mechanisms, Predictive Modeling,  
and Novel Aerospace Applications of Plasma Assisted Combustion”*

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## Plasma Flow Reactor

### Air Plasma



- self-consistent simulations of pulsed nanosecond discharges in air.
- detailed validation with experiments and analytical model results.
- demonstration of volumetric plasma heating and radical production of critical importance in combustion applications.

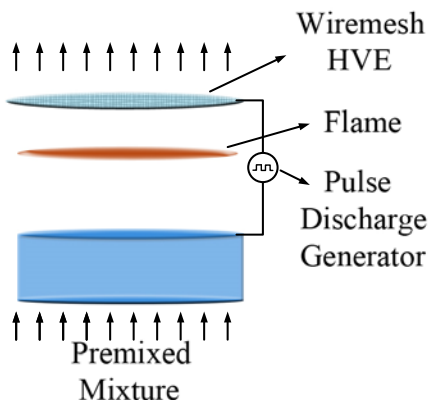
### Ignition of $H_2$ -, $CH_4$ -, and $C_2H_4$ -Air Mixtures

- critical assessment of plasma kinetic models through comparison of OH decay rates after a burst of nanosecond pulses below ignition threshold temperatures ( $\sim 500$  K).
- importance of local plasma chemistry effects over heat transport in achieving “volumetric” ignition using pulse nanosecond discharges.
- detailed parametric studies on the sensitivity of nanosecond plasma ignition to pressure, eq. ratio, pulsing frequency, burst size, initial temperature, and dielectric properties.

### Ignition of Heavy Fuels (n-Heptane)

- effect of nanosecond plasma on the two-stage n-heptane ignition process.

## Plasma-Coupled Premixed Flames



- construction of plasma flame kinetic mechanisms, including electron impact dynamics of all major species in flame environments (both reactants and products).
- effect of species and temperature gradients in the flame zone on the spatial characteristics of the plasma ( $E/N$ , electron density etc.)
- focus on plasma radical generation in the preheat zone and the impact on overall flame characteristics.

1. S. Nagaraja, V. Yang, I. Adamovich, “*Multi-Scale Modeling of Pulsed Nanosecond Dielectric Barrier Discharges in Plane-to-Plane Geometry*,” Journal of Physics D: Applied Physics 46 (15), 2013, 155205.
2. S. Nagaraja, V. Yang, Z. Yin and I. Adamovich, “*Ignition of Hydrogen-Air Mixtures using Pulsed Nanosecond Dielectric Barrier Plasma Discharges in Plane-to-Plane Geometry*,” Combustion and Flame, 2013, in press
3. S. Nagaraja, and V. Yang, “*Detailed Comparison between Nanosecond Plasma and Thermal Ignition of Hydrogen-Air Mixtures*” to be submitted to Combustion and Flame.
4. S. Nagaraja and V. Yang, “*Numerical Investigation of Nanosecond Plasma Assisted Ignition of  $H_2$ -,  $CH_4$ - and  $C_2H_4$ -Air Mixtures*” to be submitted to Combustion and Flame.
5. S. Nagaraja, W. Sun and V. Yang, “*Nanosecond Plasma Assisted Ignition of n-Heptane-Air Mixtures*,” in preparation.

## Model Assumptions

- Plasma fluid with drift-diffusion approximation.
- Two temperature model: electrons at  $T_e$  (defined using mean energy); ions and neutrals at gas temperature,  $T_{\text{gas}}$
- Lookup table for electron transport and rates using two-term expansion for electron Boltzmann equation (BOLSIG).
- Solution to mean-energy equation to update electron coefficients at each time step.
- Uniform pre-ionization in the discharge volume. No photo-ionization source term.

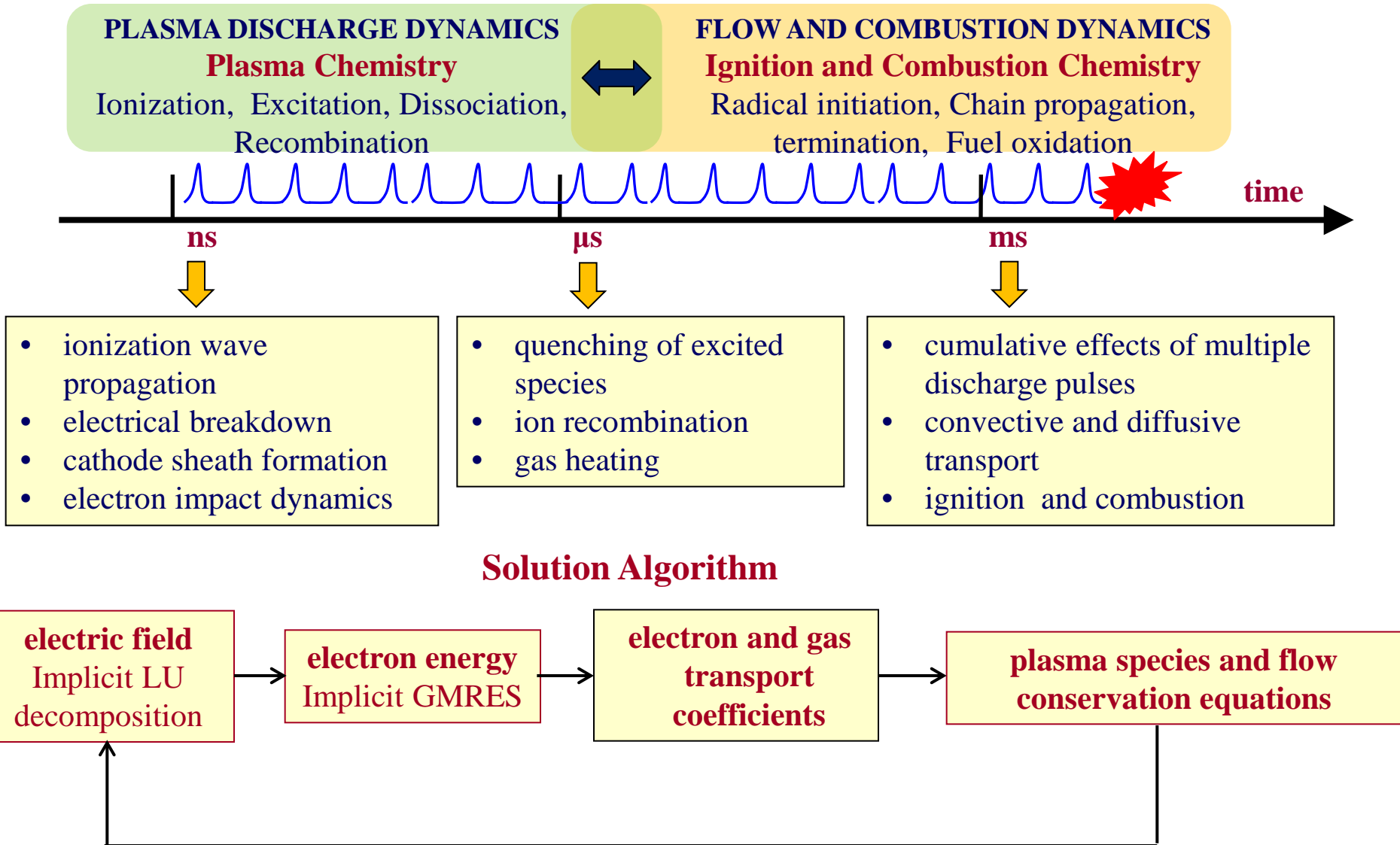
## Governing Equations

<b>Continuity</b>	$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$
<b>Momentum</b>	$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + F_i^{EHD}$
<b>Energy</b>	$\frac{\partial \rho \Omega}{\partial t} + \frac{\partial [(\rho \Omega + p) u_i]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + S_g$
<b>Species Continuity</b>	$\frac{\partial n_k}{\partial t} + \nabla \cdot \mathbf{J}_k = S_k$
<b>Equation of State</b>	$p = \sum_{i=1}^{N-1} \rho Y_i R_i T_{\text{gas}} + \rho Y_e R_e T_e$
<b>Electron Energy</b>	$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{J}_e = S_e; n_e = n_e \bar{\epsilon}$
<b>Electric Potential</b>	$\nabla \cdot (\epsilon \epsilon_0 \nabla \phi) = -e(n_+ - n_- - n_e)$
<b>Electric Field</b>	$\vec{E} = -\nabla \phi$

Validity of the BOLSIG approach to calculate electron rate coefficients, among other assumptions, has been validated through comparison of species density (O and OH), temperature and input energy with experiments

# Nanosecond Plasma Assisted Ignition and Combustion Multi-Scale Modeling Framework

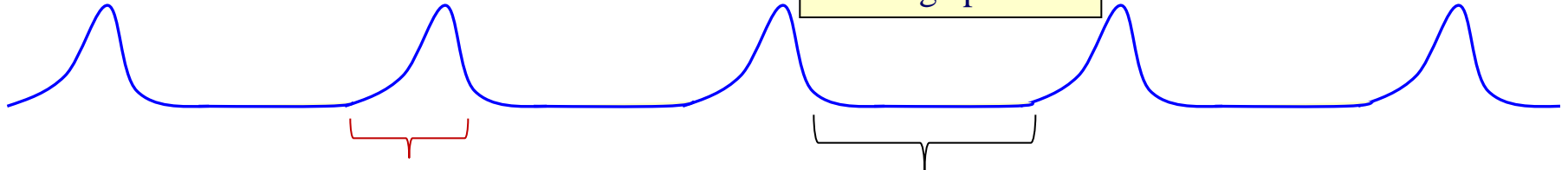
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## Adaptive Time-Stepping

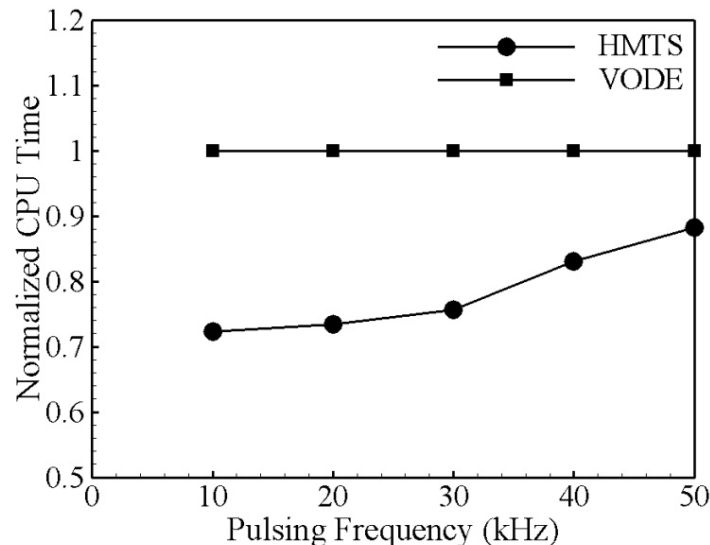
nanosecond  
voltage pulses

time gap between  
voltage pulses



- $\Delta t$  varies between  $10^{-13}$  -  $10^{-12}$  s
- Semi-implicit treatment of the Poisson equation to circumvent the stiffness arising from tight coupling between electric field and electron density.

- $\Delta t$  fixed at  $10^{-9}$  s .
- Electron energy equation and Poisson equation are not solved since electric field effects become negligible and the space charge density rapidly decay as the applied voltage ends.



## Multi Time-Scale Treatment of Chemical Source Term

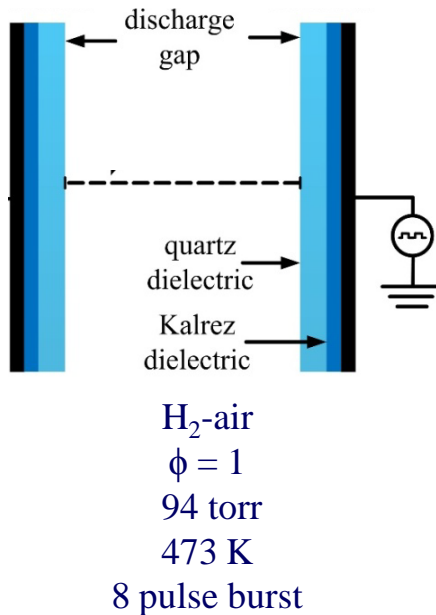
- speedup by 40% is seen by using the multi time-scale treatment of chemical source terms, but not orders of magnitude speedup observed in combustion simulations without plasma discharge.
- at high pulsing frequencies, the savings with using HMTS reduce because more time spent in simulating electric field transients during breakdown in each voltage pulse.



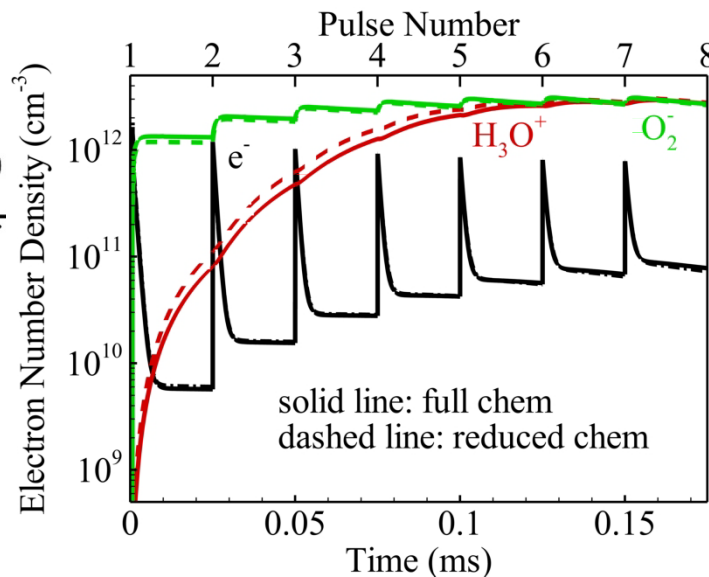
# Strategies for Computational Efficiency

## plasma combustion chemistry optimization

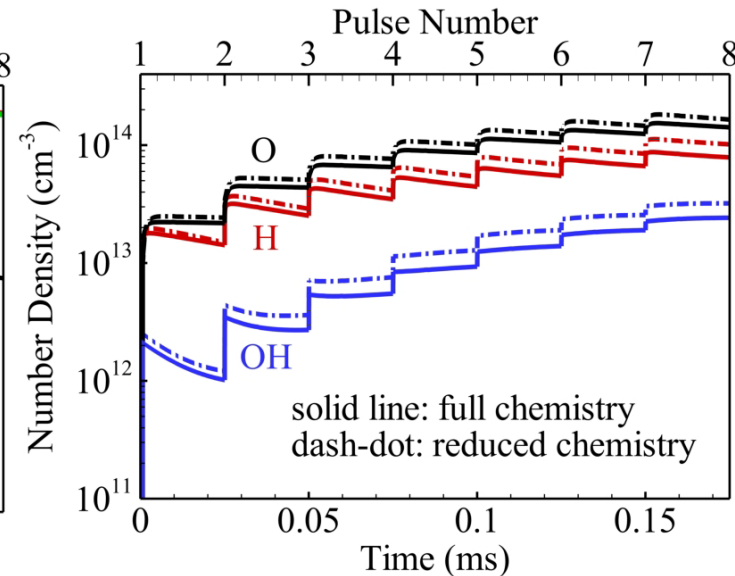
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### charged species densities at center of discharge gap



### O, H and OH densities at center of discharge gap



**full chem: 35 species, 287 reactions**

**optimized chem: 19 species 111 reactions**

- simulated a burst of 8 nanosec pulses with detailed mechanism.
- removed species with peak mole-fraction less than  $10^{-8}$
- **ensured that E/N, electron and radical species densities and temperature (in both space and time, all within 10%) are accurately predicted by the reduced mechanism.**
- provides a speed-up of  $\sim 4$  times with  $H_2$ -air plasma ignition.
- expect greater savings with large  $C_xH_y$  mechanisms and 2D/3D simulations.

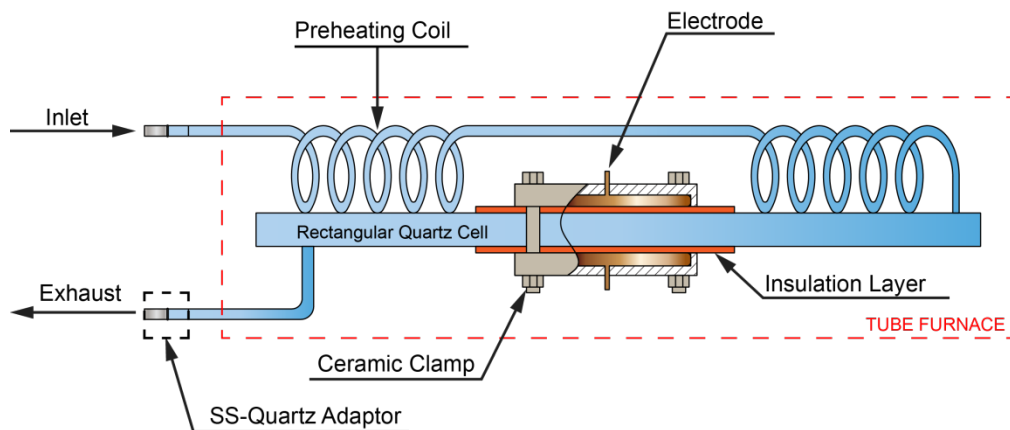


# OSU Plasma Flow Reactor

40 - 160 torr, 300 - 500 K, 1 - 100 kHz

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measurements

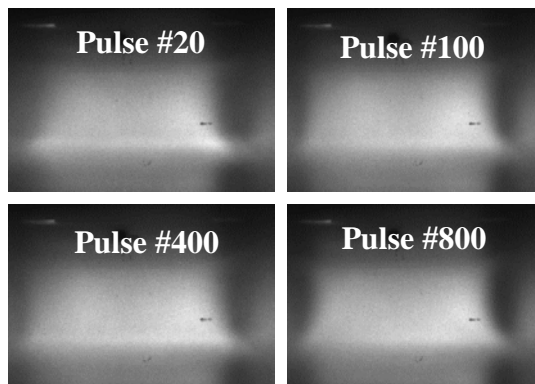


- **time resolved O density** using TALIF (uncertainty +/- 30%)
- **time resolved NO density** using LIF (uncertainty +/- 30%)
- **time resolved OH density** using LIF (uncertainty +/- 20%)
- **time resolved temperature** using rotational CARS and/or LIF thermometry
- **ignition delay time** from OH\* emission rise
- **ICCD imaging** of discharge structure and flame kernel evolution.

ICCD images of discharge structure

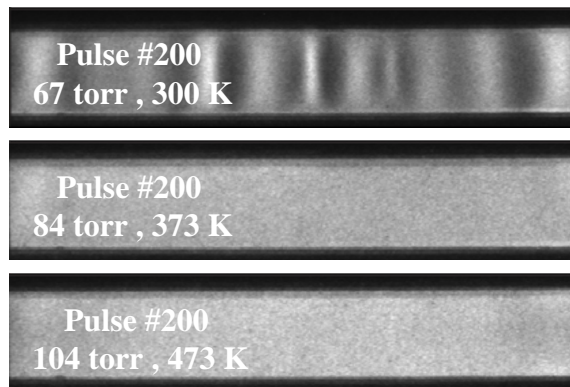
Front View (2 cm × 1 cm)

Air : 373 K, 60 torr, 40 kHz

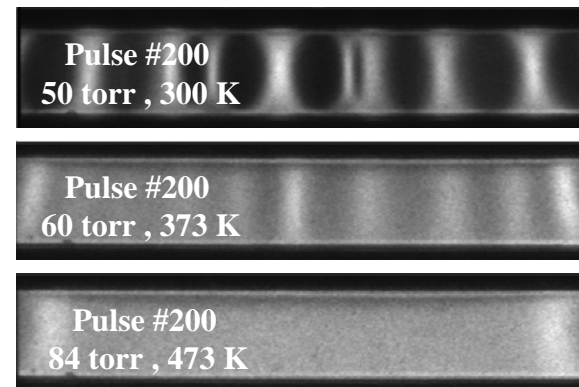


Side View (6 cm × 1 cm)

H<sub>2</sub> - Air : 40 kHz



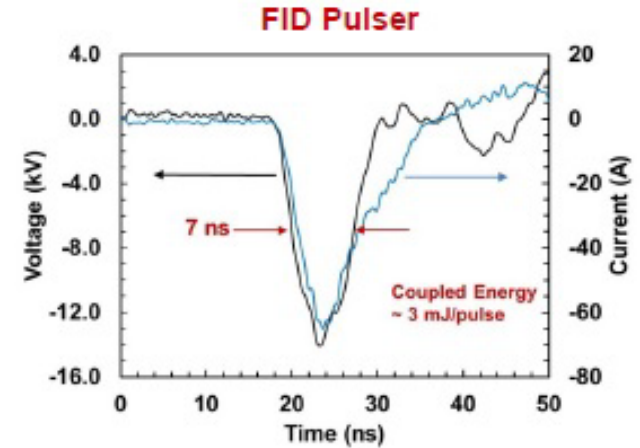
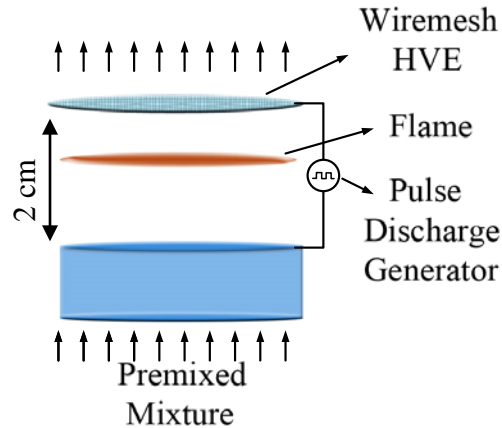
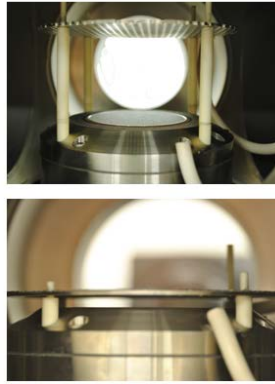
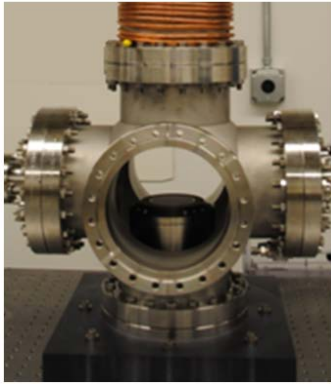
C<sub>2</sub>H<sub>4</sub> - Air : 40 kHz



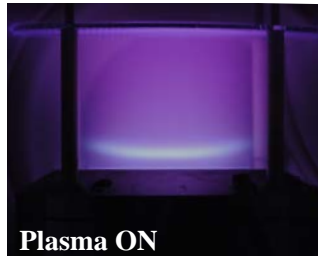
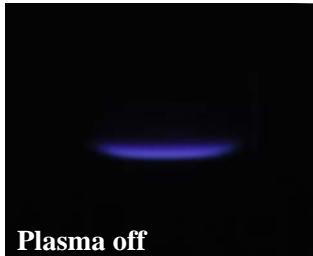
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**Burner  
Configurations**

**Facility**



**“direct coupled” configuration**



**“plasma upstream” configuration**



- low pressure 1D flame (20 - 30 torr)
- $\text{H}_2/\text{O}_2/\text{N}_2$ ,  $\text{CH}_4/\text{O}_2/\text{N}_2$  and  $\text{C}_2\text{H}_4/\text{O}_2/\text{N}_2$  premixed flames
- FID pulser: 14 kV peak voltage, 7 ns FWHM, ~3 mJ/pulse

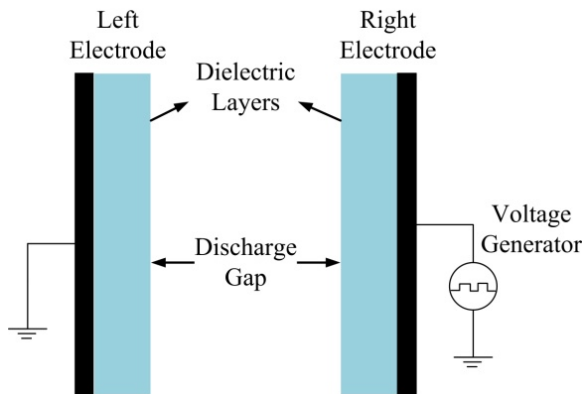
**Measurements**

- **spatially resolved OH density** using LIF
- **spatially resolved temperature** using five-line OH thermometry.

## Objectives

- Self-consistent simulations of pulsed nanosecond discharges in air with detailed kinetics.
- Validation with experiments and analytical model results.
- Direct insight into plasma heating and radical production of critical importance in combustion applications.

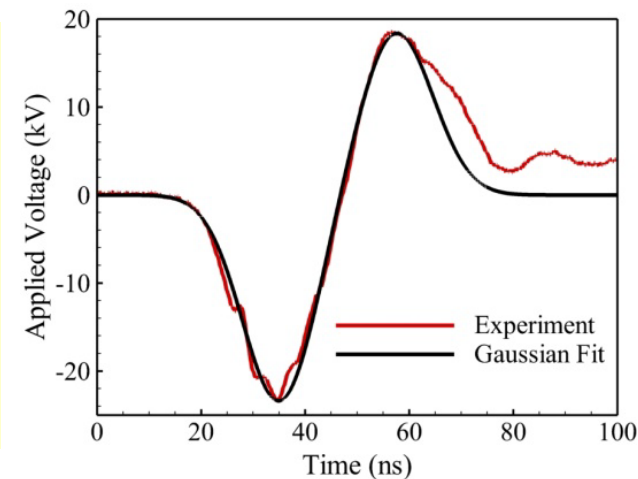
### Model Geometry



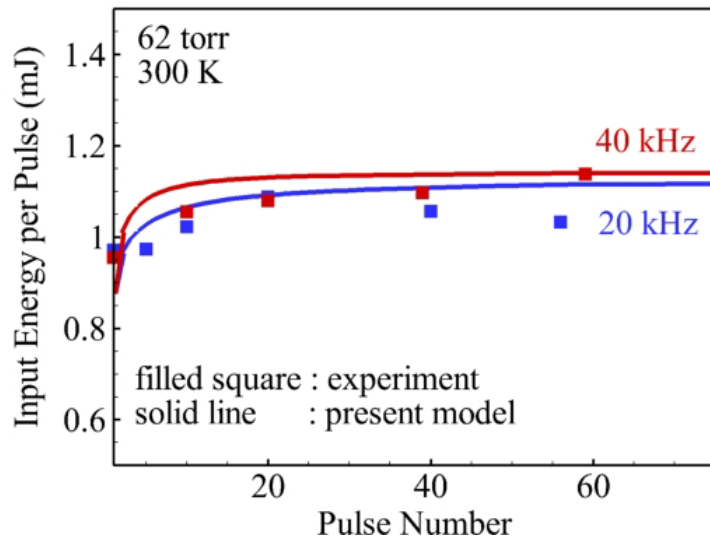
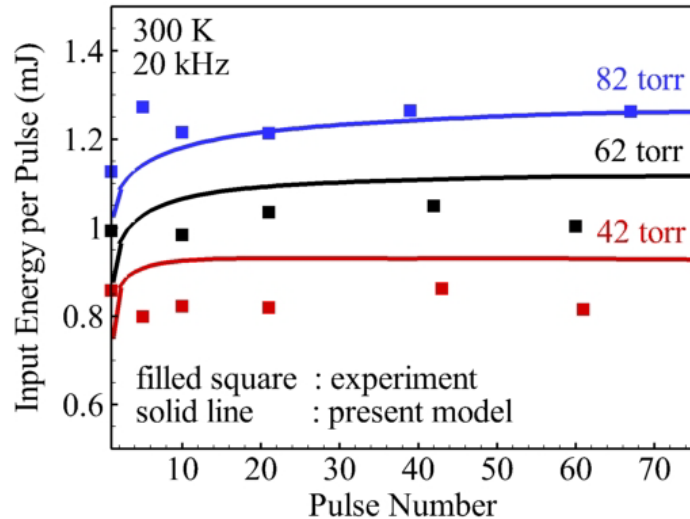
### Operating Conditions:

Initial Pressure: 60 torr  
 Initial Temperature: 300 K  
 Pulsing Frequency: 40 kHz  
 Gap width: 1 cm  
 Initial Electron Density:  $10^7 \text{ cm}^{-3}$   
 Dielectric thickness: 1.75 mm  
 Dielectric Constant: 4.3  
 Pulse Duration: 100 ns, FWHM: 12 ns  
 Peak Voltage: -22.5 kV and +17.5 kV

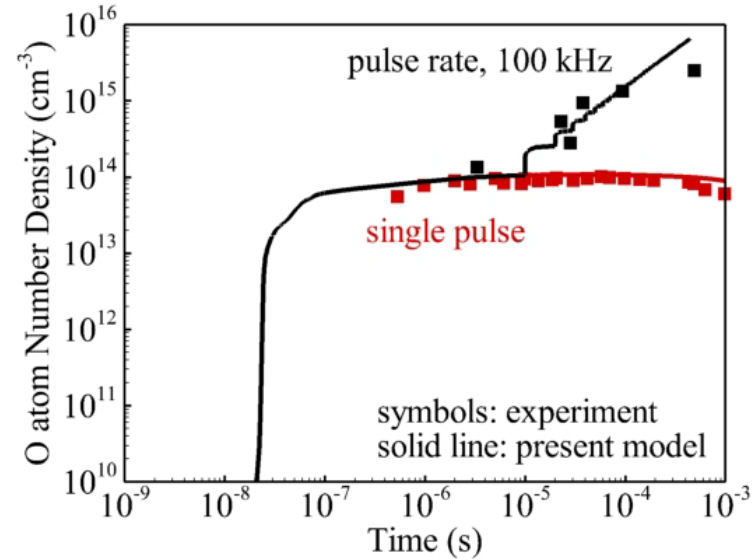
### Applied Waveform



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**Coupled Pulse Energy**



**O density at center  
of discharge volume**

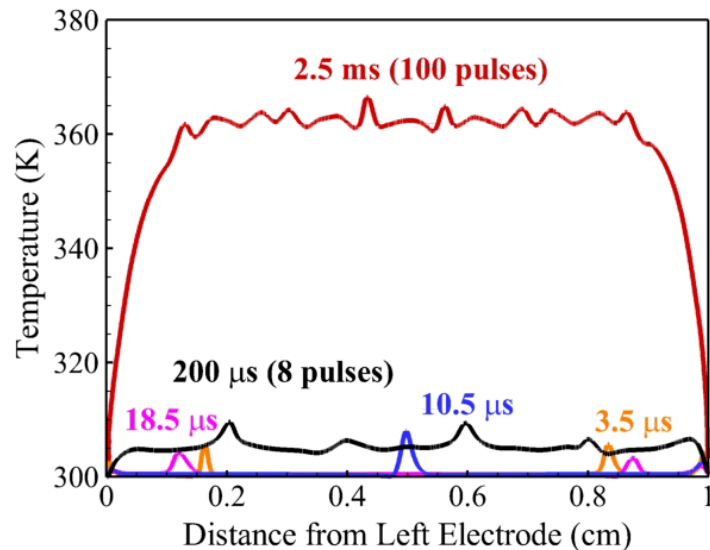


- coupled energy, temperature and O atom density predicted by the 1D model are within 20, 5 and 10% of experimental data, respectively.
- coupled energy remains fairly constant with pulse number, increasing linearly with pressure, and nearly independent of pulsing rates.
- O atom production via electron impact dissociation and quenching of excited  $\text{N}_2$  by  $\text{O}_2$  is captured accurately along with subsequent decay via formation of  $\text{O}_3$  over ms timescales.

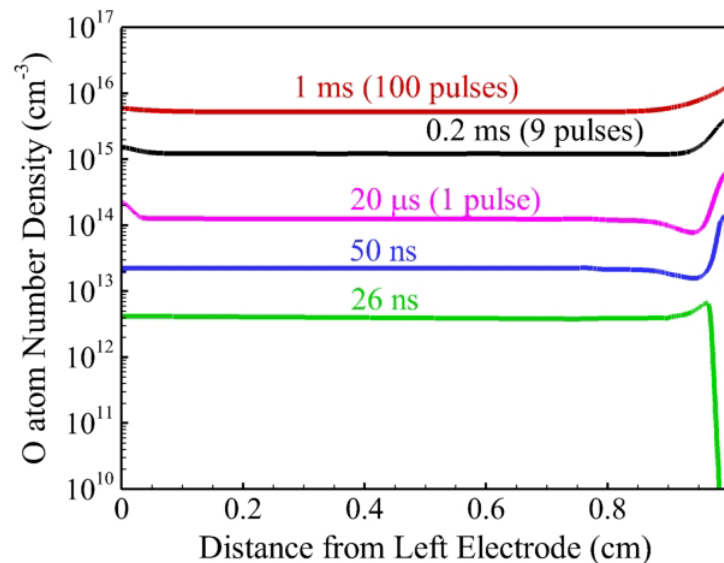
# Detailed Physics over ns-ms Timescales air discharge (60 torr, 300 K, 40 kHz, 100 pulses)

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**temperature evolution  
for 100 nanosecond pulses**



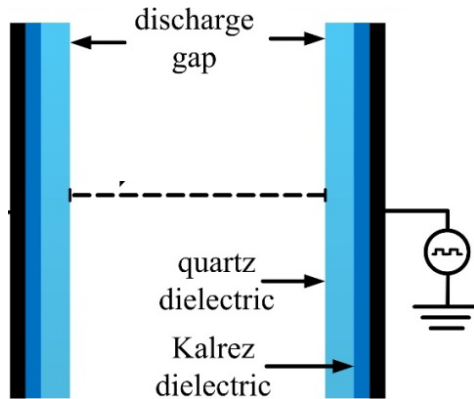
**spatial distribution of O atom density  
for 100 nanosecond pulses**



- plasma heating effect is about 0.5 - 1K/pulse in air and nearly independent of pulsing frequency (as a function of pulse number).
- rapid gas heating produces weak acoustic waves which propagate into the gas volume from both ends. The strength of these waves becomes weak as overall temperature rises from heat release from quenching of excited species.
- a fairly uniform temperature profile develops in the plasma volume after several discharge pulses, owing to slow but steady (~0.5 K/pulse) heat release primarily from relaxation of excited species.
- repetitive pulsing results in efficient production of atomic oxygen through electron impact dissociation during discharge pulses, and quenching of excited nitrogen species by oxygen.
- **volumetric radical generation and heating by pulsed discharges are of great significance for ignition and flame stabilization purposes.**



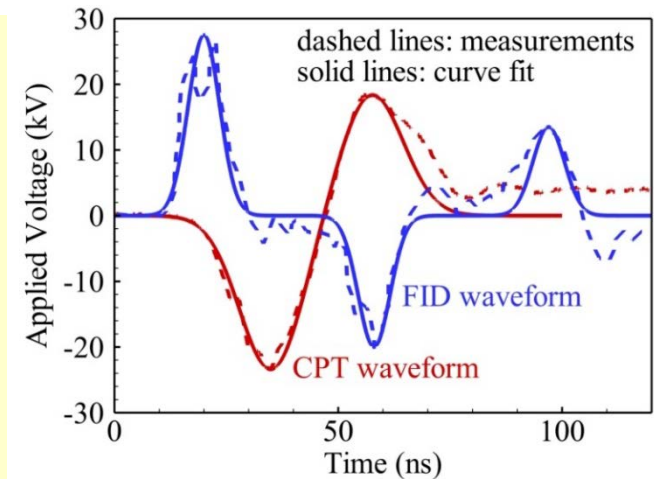
## model geometry



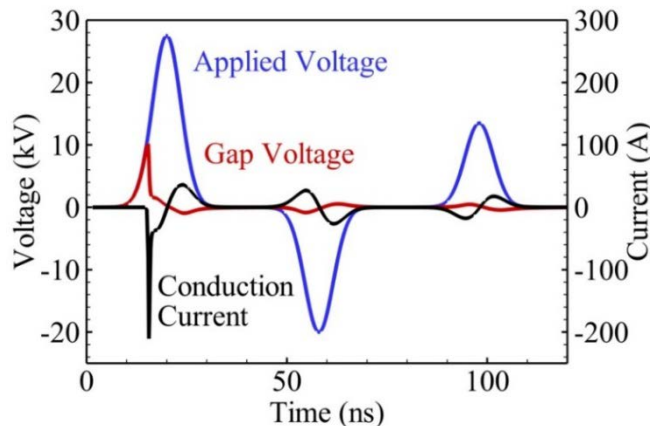
## operating conditions

Pressure: 40 - 160 torr  
Temperature: 373 - 600 K  
Pulsing Frequency: 10 - 40 kHz  
Gap width: 1 cm  
Initial Electron Density:  $10^7 \text{ cm}^{-3}$   
Dielectric thickness (Quartz): 1.75 mm  
Dielectric thickness (Kalrez): 1.58 mm  
Dielectric Constant (Quartz): 4.3  
Dielectric Constant (Kalrez): 4 - 9

## applied waveforms



## voltage and current



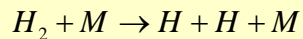
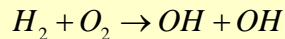
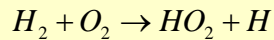
## Objectives

- comparison of OH density with measurements after a burst of 50 pulses.
- assess the accuracy of kinetics model at low temperature, pre-ignition conditions
- detailed investigations of NS plasma ignition physics and chemistry.
- sensitivity of ignition process to key system parameters and material properties.

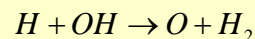
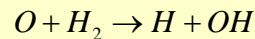
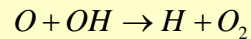
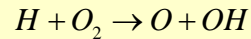
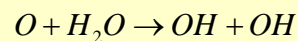
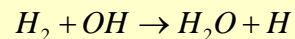
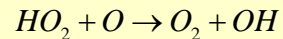
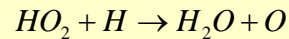
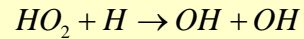
## H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> Combustion

Popov (2008) + Konnov (2008) for NOX chemistry

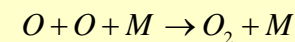
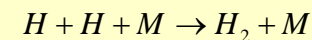
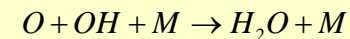
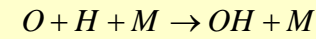
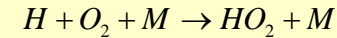
### chain initiation



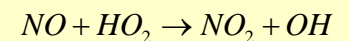
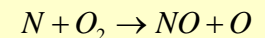
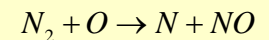
### chain branching



### three body reactions

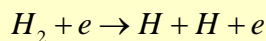
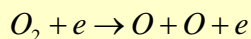
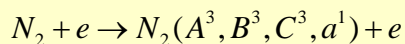
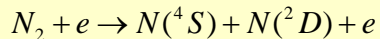


### NOX reactions

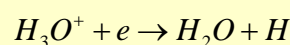
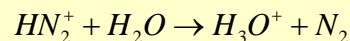
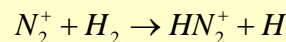
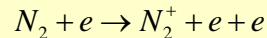


## H<sub>2</sub>/N<sub>2</sub>/O<sub>2</sub> Plasma

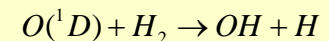
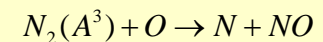
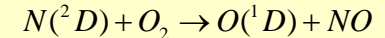
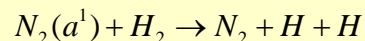
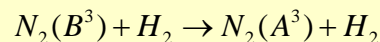
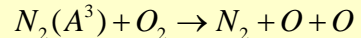
### dissociation/excitation



### ionic reactions



### quenching of excited species



nonequilibrium  
plasma chemistry



low temperature  
radical chemistry



high temperature  
combustion chemistry

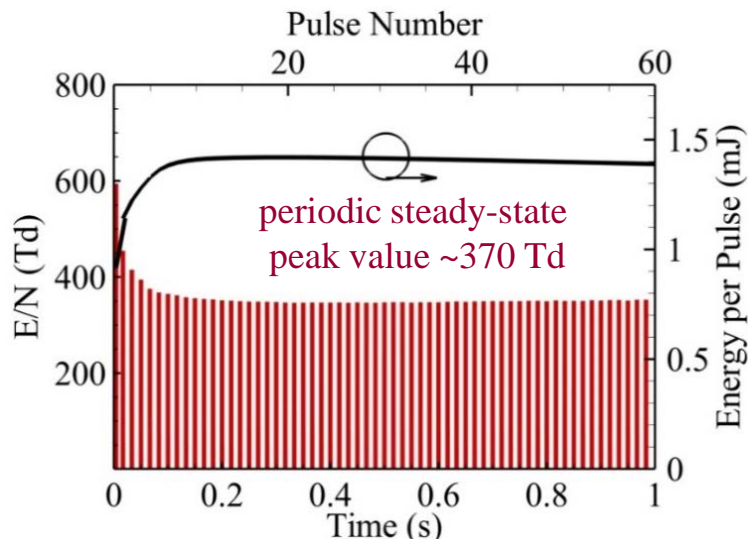
- low temperature (500-1000 K) uncertainties in many key chain branching reactions.
- detailed chemistry mechanism has 35 species and 287 reactions.
- reduced chemistry mechanism has 19 species and 111 reactions.

# E/N and Electron Density Evolution

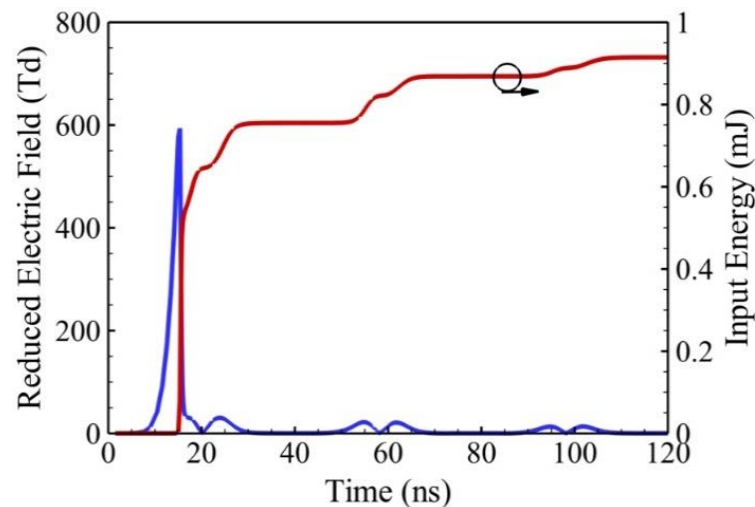
$P_i = 80$  torr,  $T_i = 500$  K,  $f = 60$  kHz,  $\Phi = 1.0$ , FID Pulser

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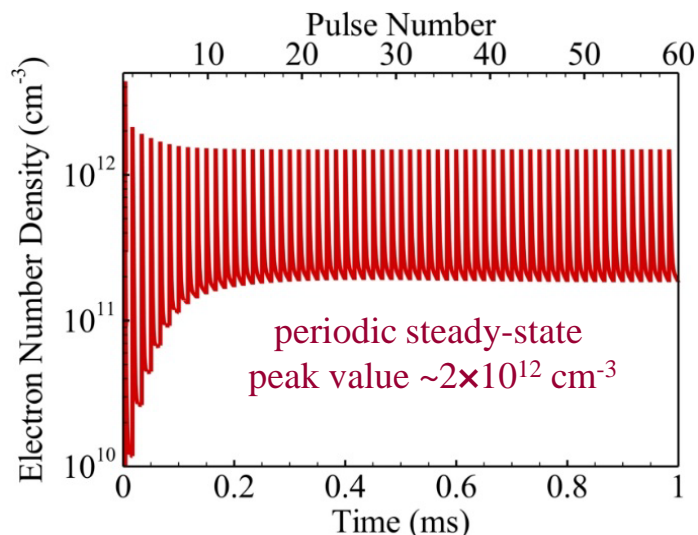
E/N at center (60 pulses)



E/N at center and input energy (first pulse)



electron density at center (60 pulses)



- breakdown voltage at these conditions occurs at  $\sim 10$  kV
- sharp spike in current is seen at breakdown before it drops rapidly from the plasma shielding.
- plasma excited species production happens only during a short duration of  $\sim 5$  ns when E/N is high.
- E/N and electron density reach a periodic steady state after  $\sim 8$  pulses.
- nanosecond discharge efficiently generates radicals and excited species during each pulse because of high peak E/N.

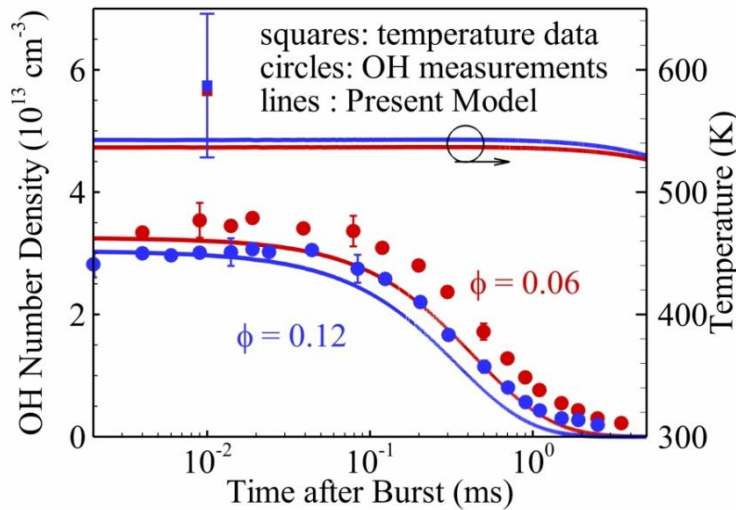


# Decay Rates of O, H and OH after a 50 pulse burst in H<sub>2</sub>-air

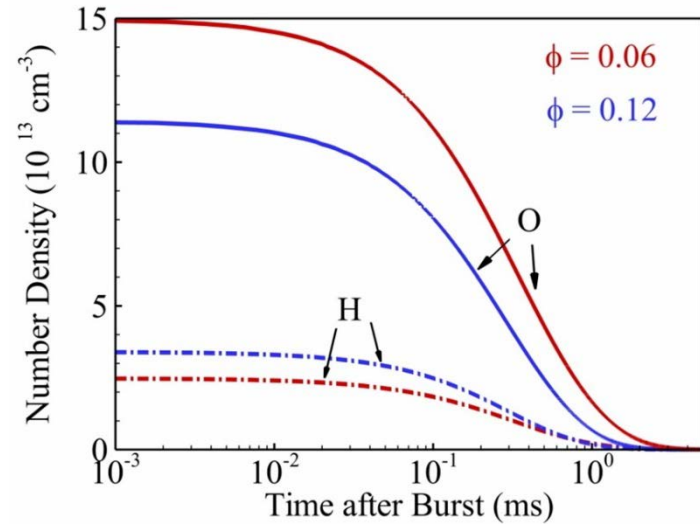
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$P_i = 100$  torr,  $T_i = 500$  K,  $f = 10$  kHz, FID pulser

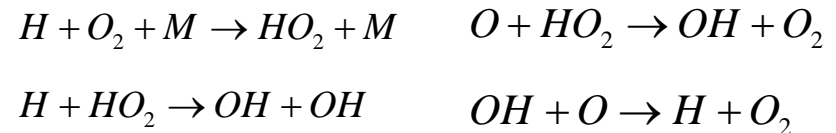
OH density at center of discharge gap



O and H density at center of discharge gap



key low temperature pathways for consumption of O and recirculation of H and OH

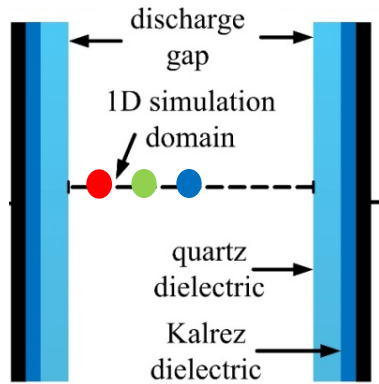


- model predictions for OH are within 10% of measurements in H<sub>2</sub>-air mixtures, including both peak value and decay rates.
- O production is highly sensitive to changes in eq. ratio, increasing by ~50% when  $\phi$  is decreased from 0.12 to 0.06.
- H and OH are relatively insensitive, changing by ~10 % when eq. ratio is doubled.

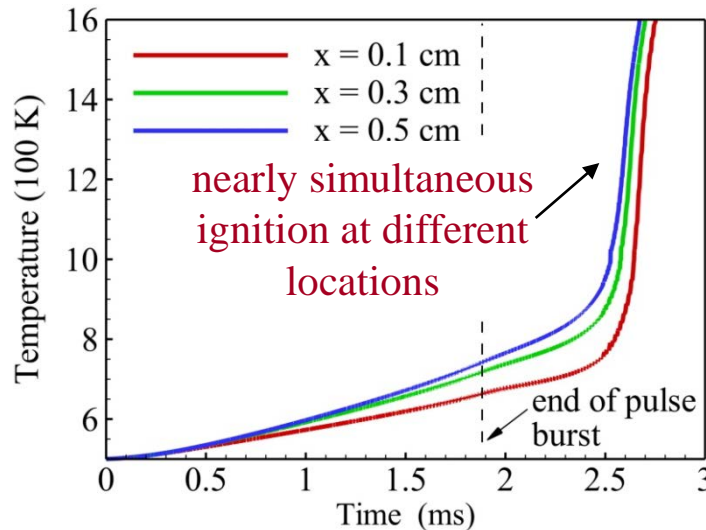
# How is ignition achieved with nanosecond plasma?

$P_i = 80$  torr,  $T_i = 500$  K,  $f = 60$  kHz,  $\Phi = 1.0$ , FID pulser, 115 pulses  $\sim 2$  ms

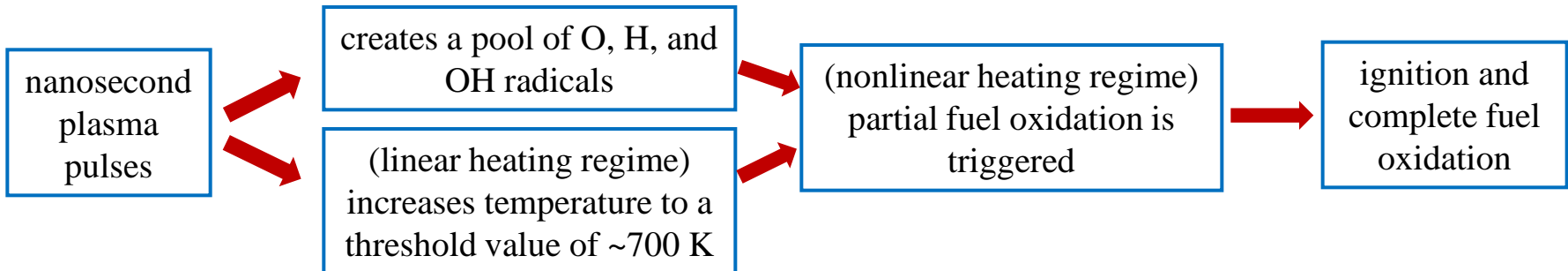
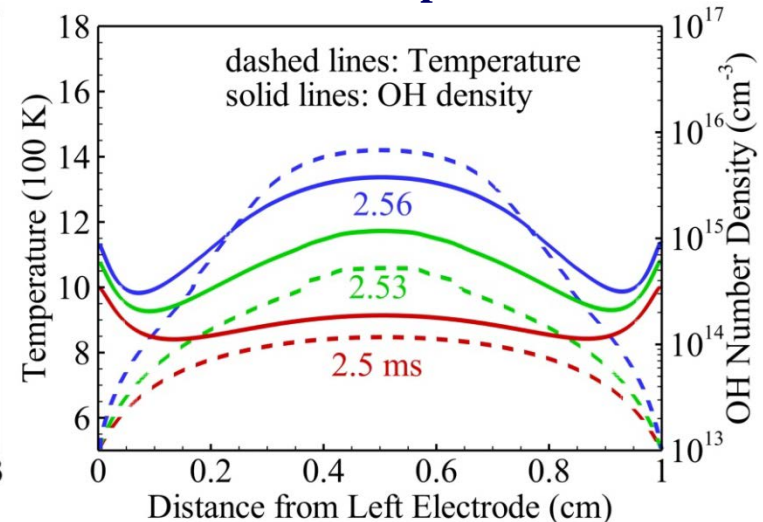
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**temperature evolution vs time**



**spatial evolution of OH and temperature**



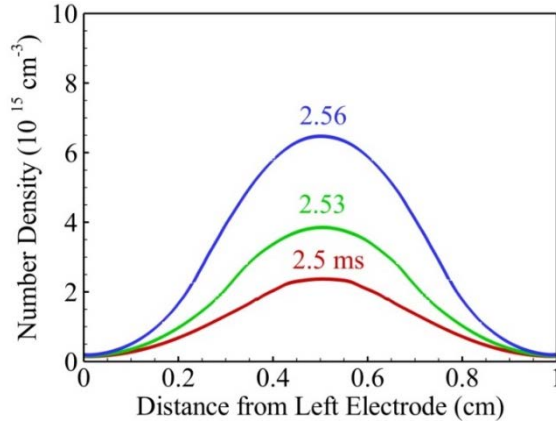
- heat transport plays a minor role. local plasma chemistry effects are critical in producing “volumetric” ignition
- secondary peaks in OH density near the boundaries is generated from  $\text{HO}_2$  which has accumulated due to low temperatures

# Spatial Evolution of Radicals during H<sub>2</sub>-Air Ignition

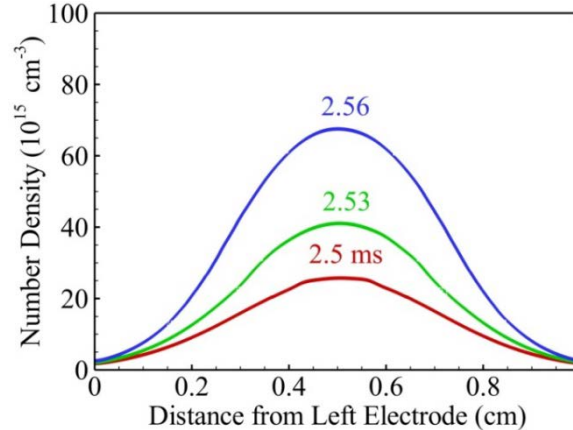
$P_i = 80$  torr,  $T_i = 500$  K,  $f = 60$  kHz,  $\Phi = 1.0$ , FID pulser, 115 pulses  $\sim 2$  ms

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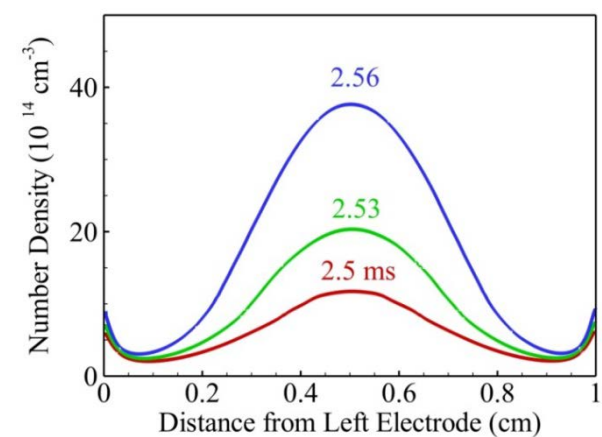
**O**



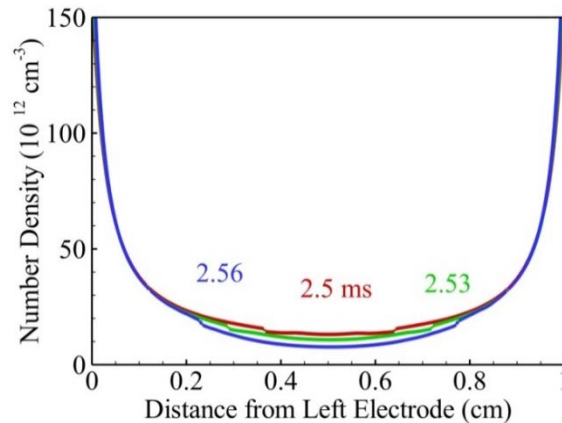
**H**



**OH**



**HO<sub>2</sub>**



- a small increase in temperature near ignition significantly increases the chain branching reaction rates.
- radical concentration profiles are much steeper than the temperature distribution, with well pronounced maxima near the centerline.
- both O and H densities increase by  $\sim 3$  times within 0.4 ms near ignition, with OH density increasing by 4 times.
- low temperatures at the boundaries because of heat losses aid the accumulation of HO<sub>2</sub> which generates OH. The secondary peaks in OH profiles near the boundaries result from this pathway.

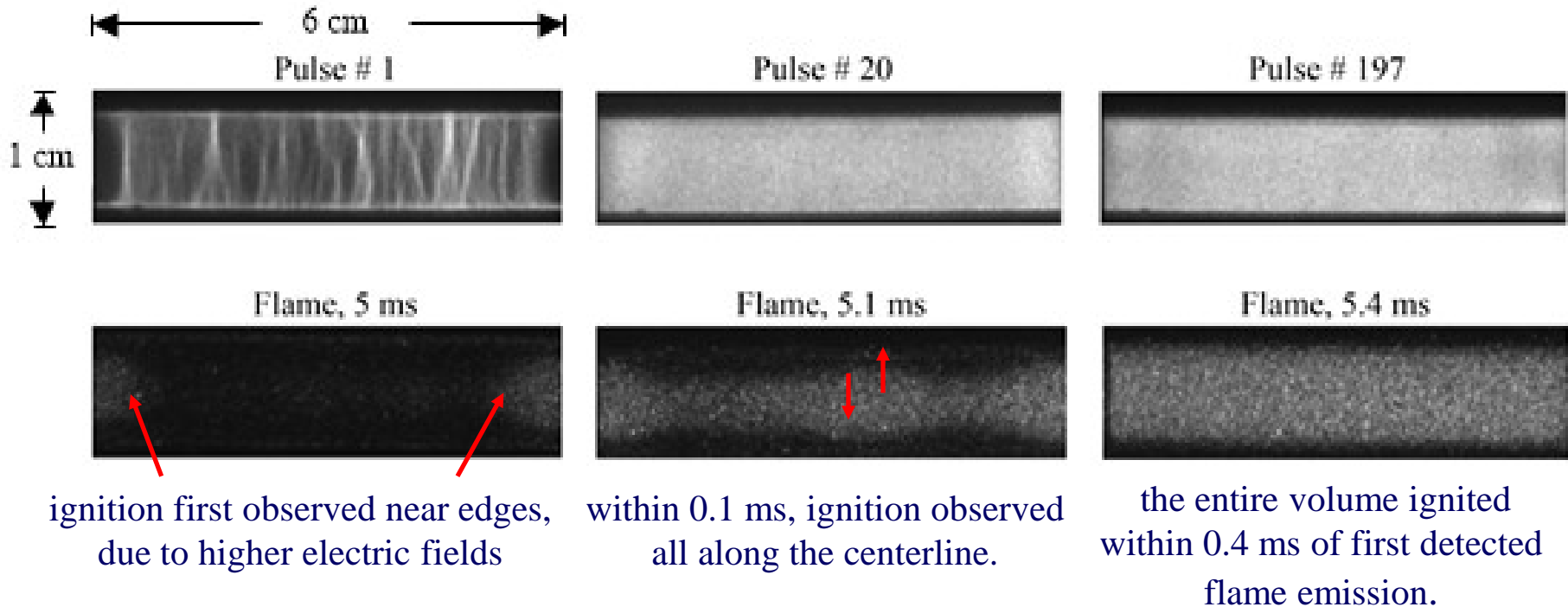
# H<sub>2</sub>-air pulsed nanosecond plasma ignition

## what can we infer from emission images?

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### OSU Experiment

$P_i = 104$  torr,  $T_i = 473$  K,  $f = 40$  kHz,  $\Phi = 1.0$ , CPT pulser



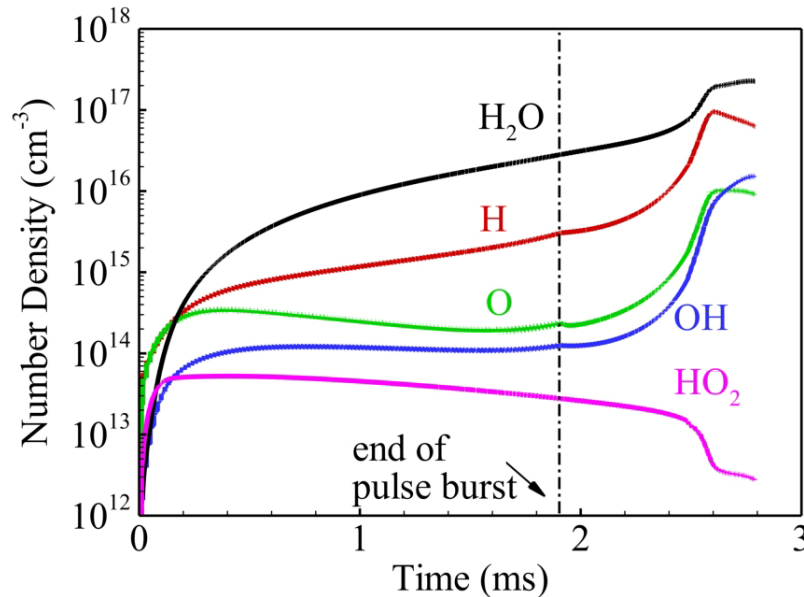
- the present 1D model simulates a particular cross-section.
- although the 1D model cannot capture edge effects, it is able to explain the spreading of the ignition kernel from the centerline towards the boundaries.
- predictions are in line with observations that local plasma chemistry dominate over heat transport effects

# Nanosecond Plasma Ignition vs Thermal Ignition

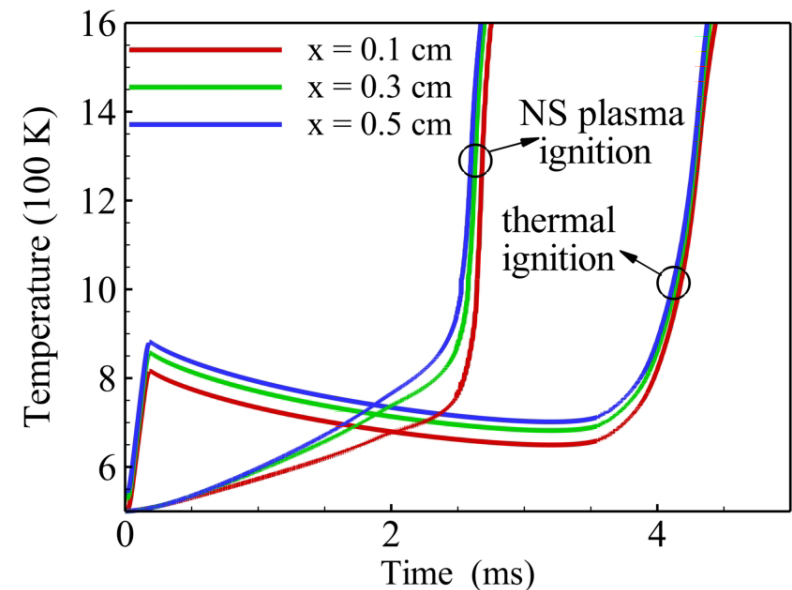
## is there any difference?

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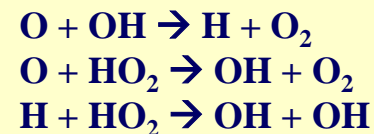
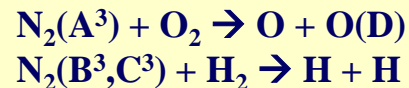
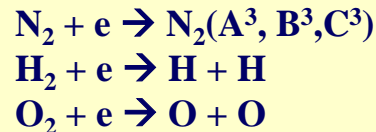
species evolution at center for  
NS ignition



ignition delay times with nanosecond  
plasma and a volume heat source



steps in the nanosecond plasma ignition process

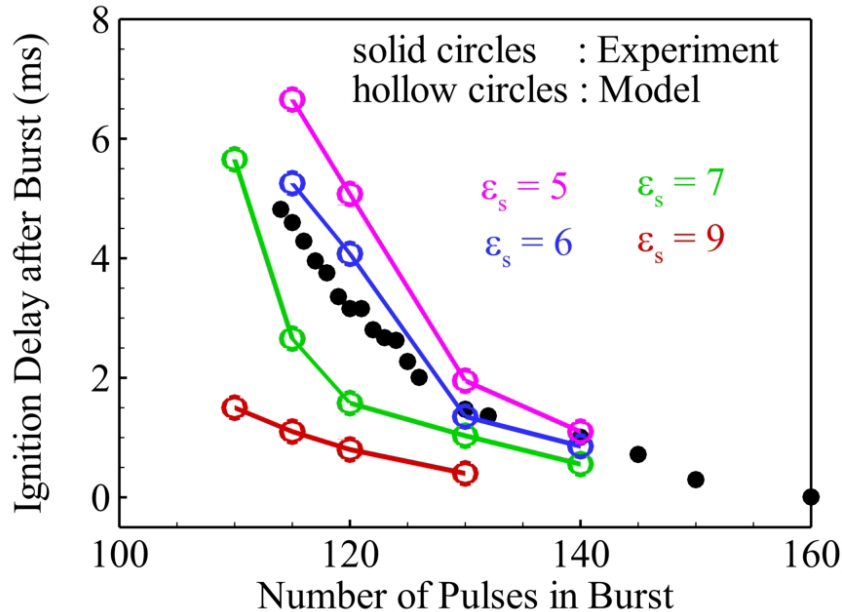


- the high activation energy chain initiation reactions are replaced by electron impact reactions with NS plasma.
- for the same input energy, thermal ignition delay is ~ 60% higher.
- plasma generated radicals trigger heat release from fuel oxidation at ~700 K, as opposed to auto-ignition temperature of ~960 K under same conditions.

## ignition delay vs # pulses in burst

$P_i = 80$  torr,  $T_i = 473$  K

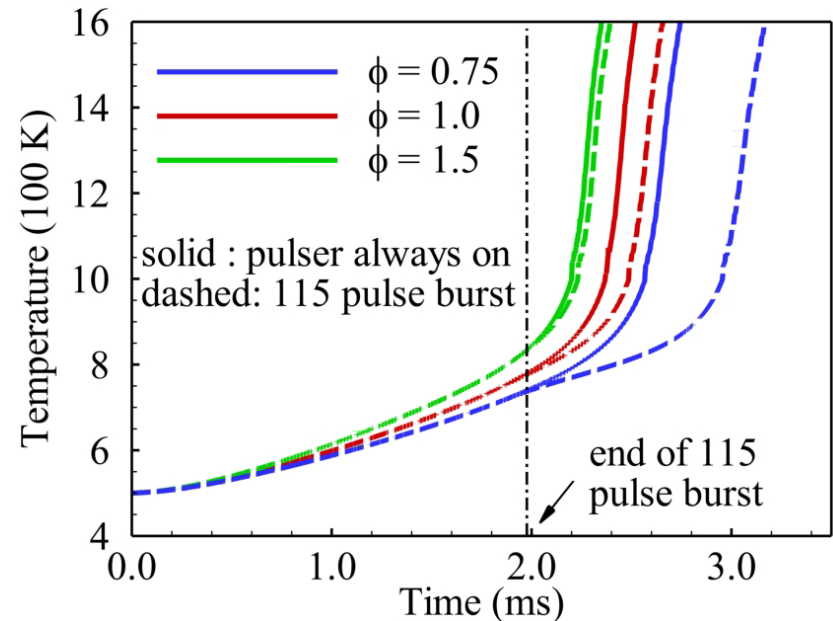
$f = 40$  kHz,  $\Phi = 1.0$ , CPT pulser



## ignition delay sensitivity to eq. ratio

$P_i = 80$  torr,  $T_i = 500$  K

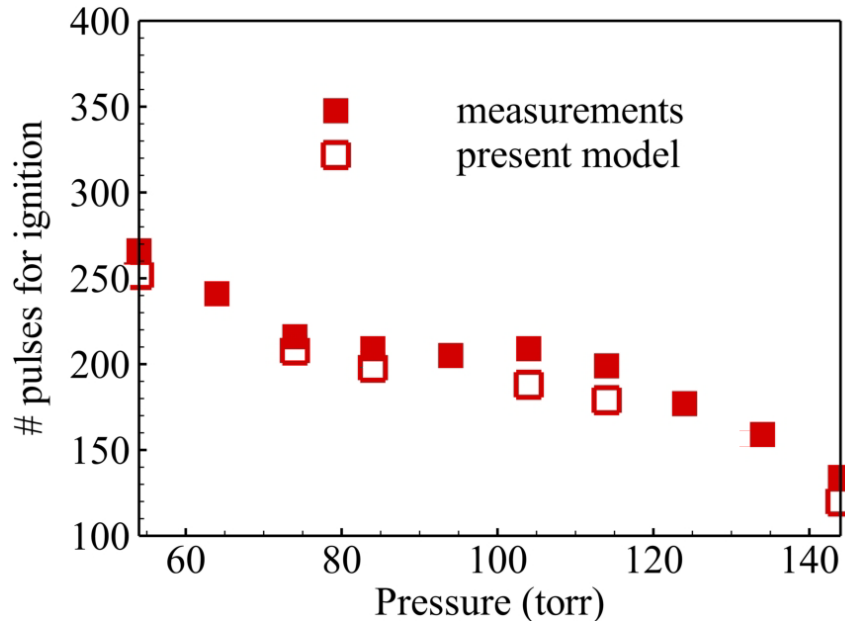
$f = 60$  kHz, FID pulser



- there is a minimum # of pulses in burst, below which no ignition is observed.
- ignition characteristics are highly sensitive to dielectric properties.
- uncertainty in the dielectric constant values should be considered during the validation process.
- ignition delay reduction with increase in burst size is especially pronounced for lean mixtures.



$T_i = 473 \text{ K}$ ,  $f = 40 \text{ kHz}$ ,  $\phi = 1.0$ , CPT pulser



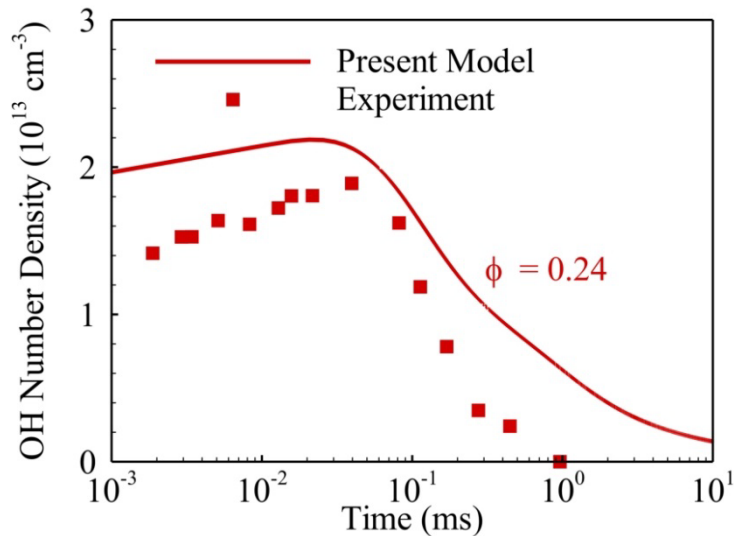
- ignition delay reduction with increase in pressure is well reproduced by the model.
- increase in pressure results in nearly linear rise in input energy per pulse because of its dependence on number density. Faster addition of energy results in more rapid ignition at higher pressures.
- the nonlinear trend of # pulses required for ignition as a function of pulsing frequency is not reproduced by the model.
- the model predicts that input energy per pulse is nearly independent of pulsing frequency, which may not be true.
- lowering of input energy, because of residual electron density effects, with rise in pulsing rates may explain the observed nonlinear trend.

# OH Density Decay after 50 Pulse Burst in CH<sub>4</sub>-, and C<sub>2</sub>H<sub>4</sub>-Air Mixtures

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$P_i = 100$  torr,  $T_i = 500$  K,  $f = 10$  kHz, FID pulser

**CH<sub>4</sub>-air**



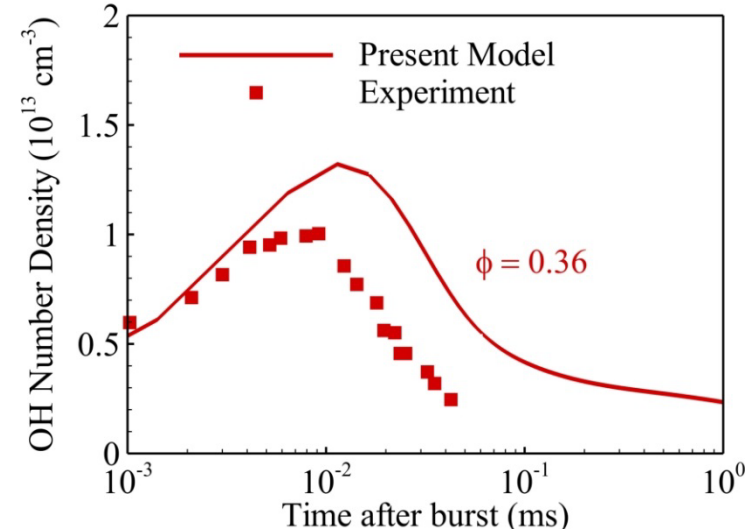
**CH<sub>4</sub>-air  
(64 species)**

GRI Mech 3.0  
CH<sub>4</sub>/N<sub>2</sub>/O<sub>2</sub> plasma  
NOX reactions

**C<sub>2</sub>H<sub>4</sub>-air  
(70 species)**

USC Mech  
C<sub>2</sub>H<sub>4</sub>/N<sub>2</sub>/O<sub>2</sub> plasma  
NOX reactions

**C<sub>2</sub>H<sub>4</sub>-air**

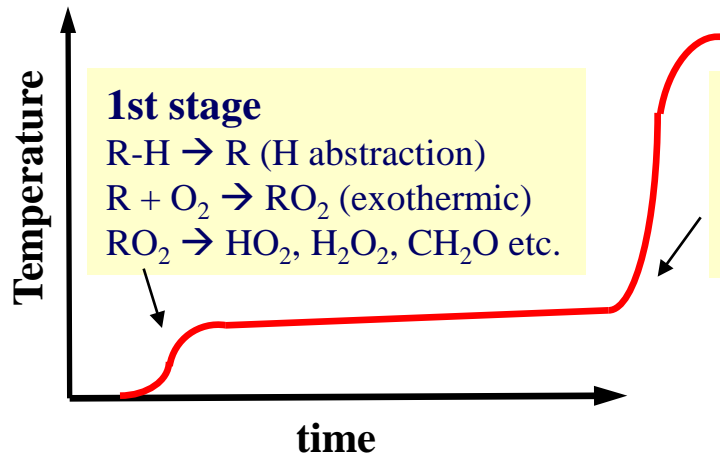


- GRI Mech 3.0 has been validated extensively in 1000-2500 K and 25 torr to 10 atm range.
- USC Mech has been validated in 900-2500 K and 16 torr to 10 atm range.
- model consistently over-predicts OH density by ~50% in CH<sub>4</sub>-air mixtures.
- growth rate is correctly predicted in C<sub>2</sub>H<sub>4</sub>-air mixtures, but the decay rate is slower than measurements.
- low temperature uncertainty in chain reactions may be the primary reason for deviations

## Ongoing Work

- different CH<sub>4</sub>- and C<sub>2</sub>H<sub>4</sub>-air combustion chemistry integrated with plasma kinetics are being tested to assess their relative performance on predicting low temperature radical production/decay.



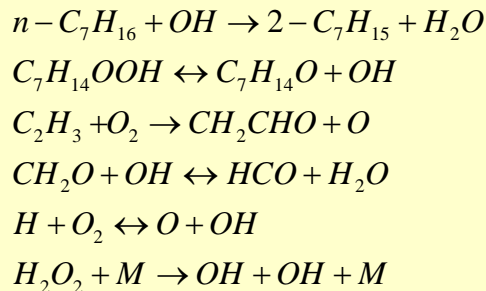


## Objective

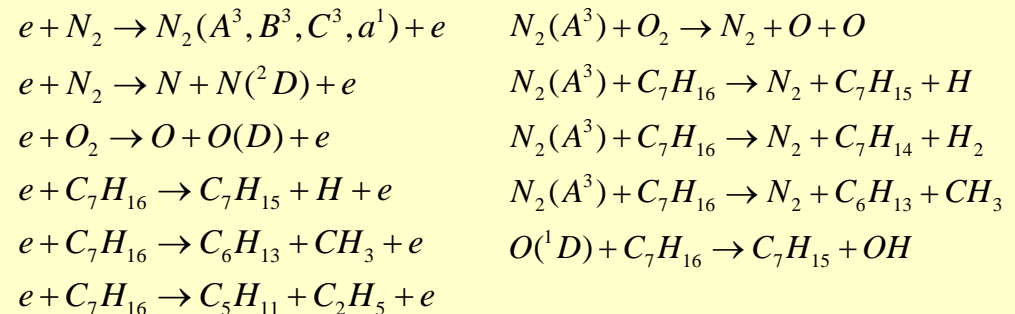
- understand the effect of NS plasma on n-heptane-air ignition chemistry through self-consistent simulations.
- investigate the effect of radical addition to the “low temperature” and “high temperature” steps of the 2-stage ignition process.

## nC<sub>7</sub>H<sub>16</sub>-air plasma combustion kinetics (154 species)

### C<sub>7</sub>H<sub>16</sub>/N<sub>2</sub>/O<sub>2</sub> combustion (LLNL reduced mech + NOX reactions)



### C<sub>7</sub>H<sub>16</sub>/N<sub>2</sub>/O<sub>2</sub> plasma reactions\*

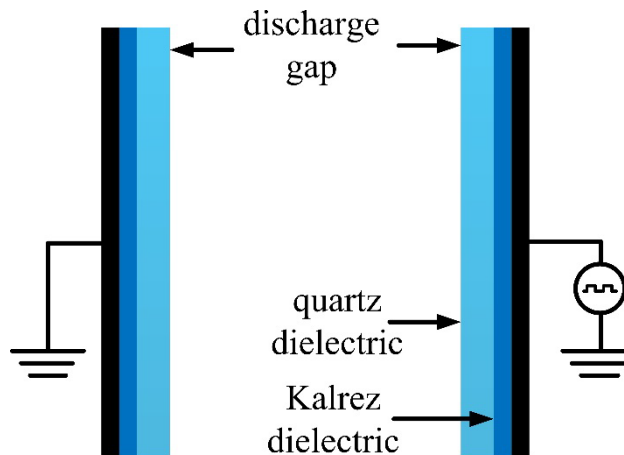


\* C<sub>7</sub>H<sub>16</sub> (electron impact and with excited species) reaction rates estimated from C<sub>3</sub>H<sub>8</sub> based plasma reactions.

# Nanosecond Plasma Ignition of nHeptane-Air

## Effect of NS Pulses on 1st Stage Delay Time

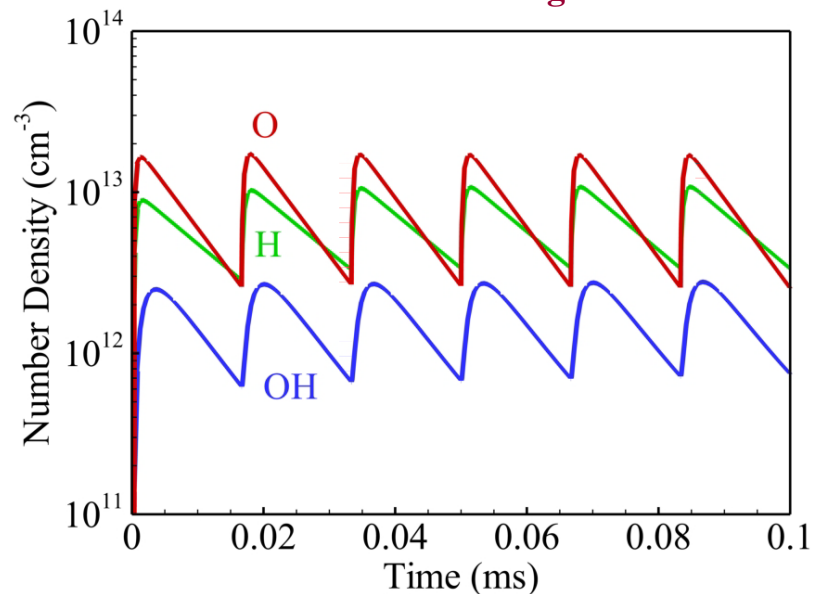
### School of Aerospace Engineering model geometry



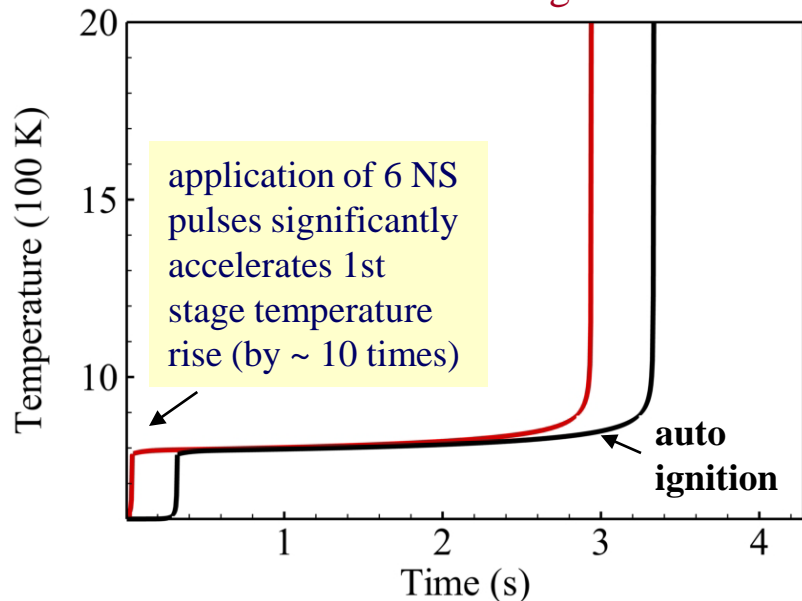
### operating conditions

$P_i = 160$  torr  
 $T_i = 600$  K  
 $f = 60$  kHz  
 $\Phi = 1.0$   
8 kV Gaussian pulses  
10 ns duration

### O, H and OH density evolution at center of discharge volume



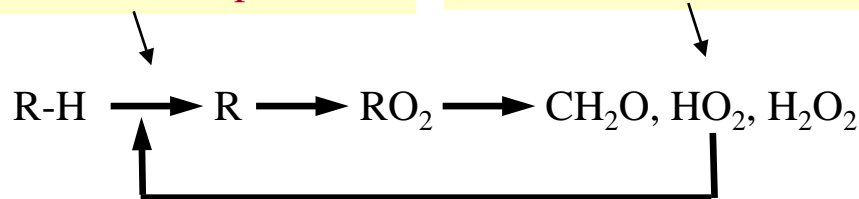
### temperature evolution at center of discharge volume



### “self-acceleration” of low temperature chemistry

addition of small amount of radicals accelerates the H abstraction step

$\text{RO}_2$  produces more radicals which accelerate the whole process further.



# Nanosecond Plasma Ignition of nHeptane-Air

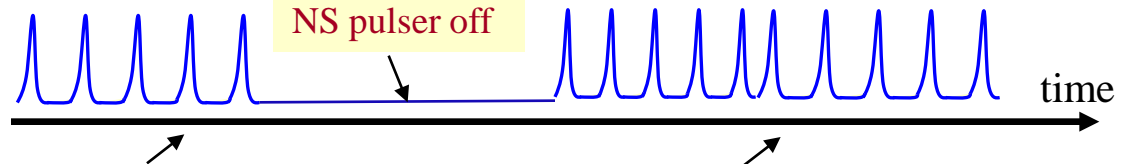
## Effect of NS Pulses on Overall Ignition Delay Time

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### operating conditions

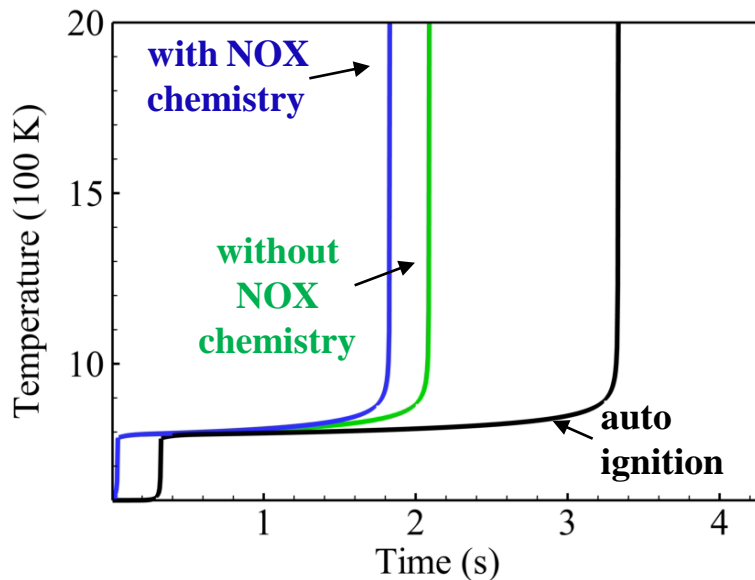
$P_i = 160$  torr  
 $T_i = 600$  K  
 $f = 60$  kHz  
 $\Phi = 1.0$   
 8 kV Gaussian pulses  
 10 ns duration

### “staggered” application of NS pulses



only a few NS pulses  
sufficient to rapidly trigger  
1st stage temperature rise

25 NS pulses are applied after  
the 1st stage to reduce the  
overall ignition delay



- the “staggered” application of NS pulses result in ~ 40% reduction in ignition delay time
- it is evident that the 2nd stage is less sensitive to radical addition by NS pulses than the 1st stage.
- heating provided by the NS pulses after the 1st stage accelerate the decomposition of  $\text{H}_2\text{O}_2$  and reduce ignition delay.



- inclusion of NOX catalytic reactions change the predictions by ~5% because of following new OH generation pathways.

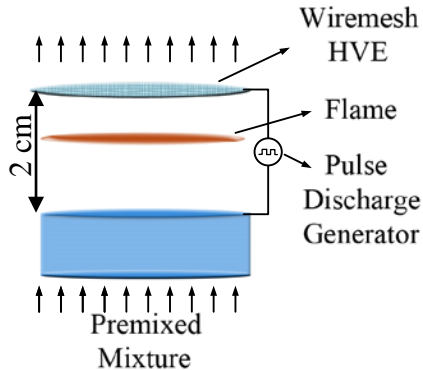


# Nanosecond plasma coupled premixed flame

## CH<sub>4</sub>-air

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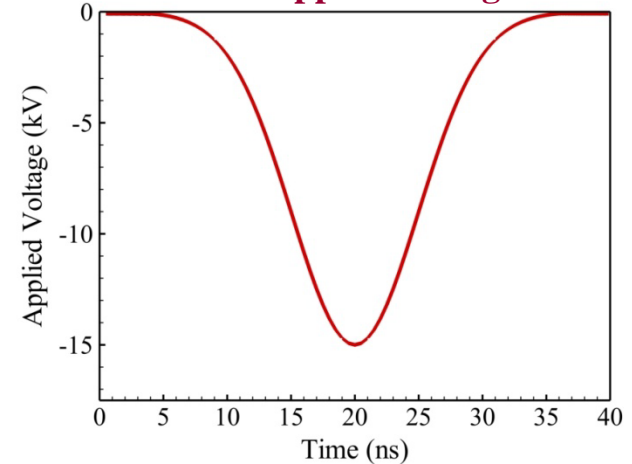
#### physical setup



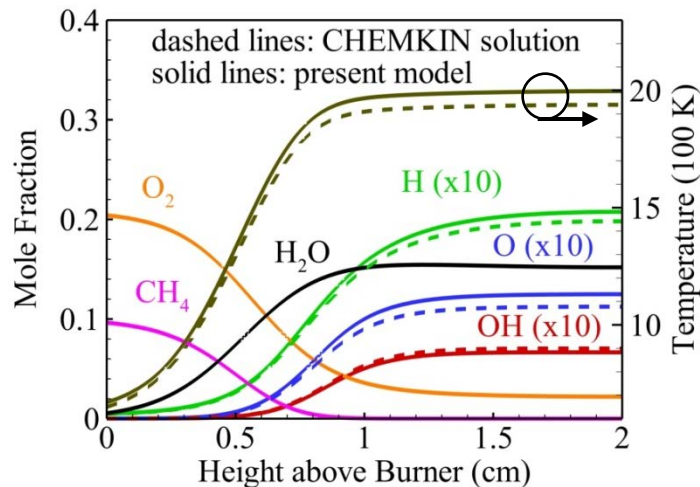
#### operating conditions

Pressure: 25 torr  
 Inlet Temperature: 650 K  
 Eq. ratio: 1.07  
 Gap width: 4.0 cm  
 initial Electron Density:  $10^7 \text{ cm}^{-3}$   
 -15 kV peak voltage  
 7 ns FWHM  
 $\dot{m}$  :  $0.00377 \text{ kg/m}^2\text{-s}$

#### applied voltage



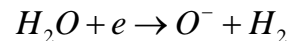
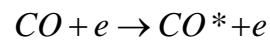
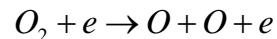
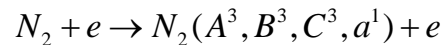
#### validation of flame model with CHEMKIN solution



#### CH<sub>4</sub>-air plasma flame kinetics (75 species)

GRI Mech 3.0 + CH<sub>4</sub>/N<sub>2</sub>/O<sub>2</sub>/CO/CO<sub>2</sub> plasma + NOX chemistry

- electron impact processes of both reactant (CH<sub>4</sub>, O<sub>2</sub>, N<sub>2</sub>) and product species (H<sub>2</sub>O, CO, CO<sub>2</sub>) considered.



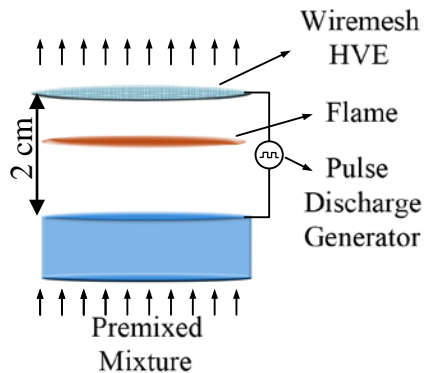
- what are most important plasma pathways pertaining to H<sub>2</sub>O, CO, CO<sub>2</sub> ?
- is plasma species production in preheat zone more important than downstream?

# Plasma Coupled Premixed CH<sub>4</sub>-Air Flame

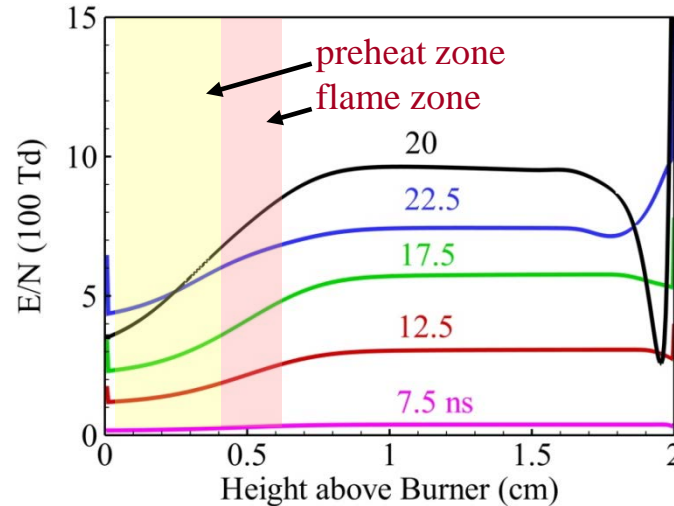
$$P_i = 25 \text{ torr}, T_i = 650 \text{ K}, \Phi = 1.07$$

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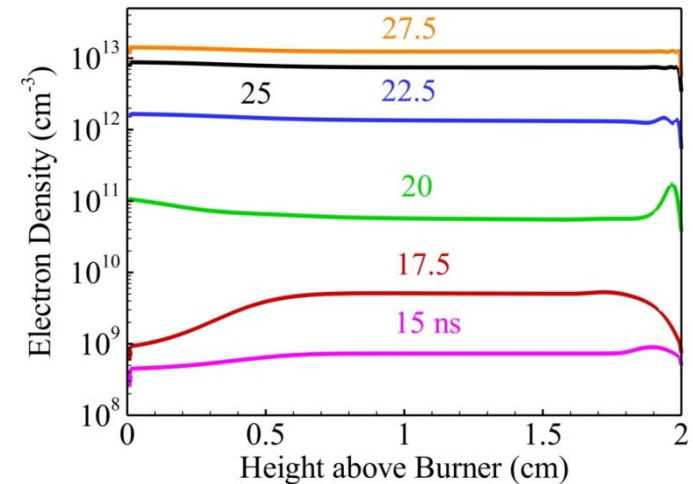
## physical setup



## reduced electric field vs height



## electron density vs height



high E/N (100 - 600 Td) and high electron densities ( $\sim 1e13 \text{ cm}^{-3}$ ) allow for efficient radical generation by NS pulses in preheat zone, where they may provide significant benefit.

note that radicals (O, H, OH etc) concentration in the flame zone is already of the order 10,000 ppm, so plasma cannot make much impact

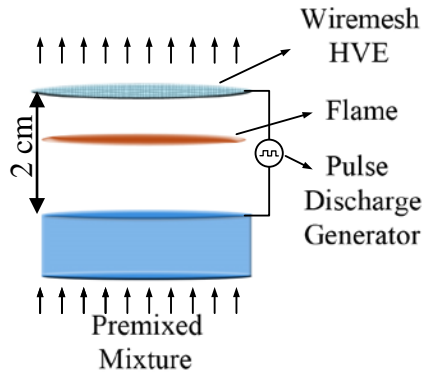
- high E/N downstream of the flame can be attributed to high temperatures and low number density.
- E/N in the preheat zone reaches  $\sim 600 \text{ Td}$  at 22.5 ns. Plasma radical generation in this zone may have a significant impact on flame characteristics.
- sharp peak in the E/N profile at 20 ns at the right boundary indicates the cathode sheath region.
- electron density distribution is fairly uniform in the entire domain reaching peak value of  $2 \times 10^{13} \text{ cm}^{-3}$  at 27.5 ns.
- total input energy during the pulse was 2.7 mJ

# Plasma Coupled Premixed CH<sub>4</sub> - Air Flame

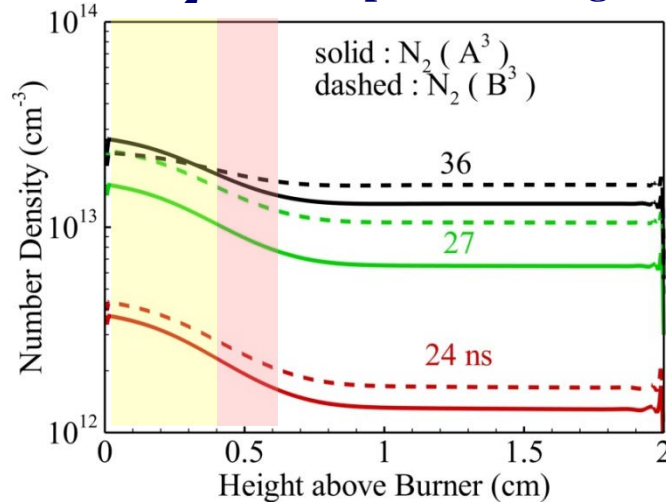
$$P_i = 25 \text{ torr}, T_i = 650 \text{ K}, \Phi = 1.07$$

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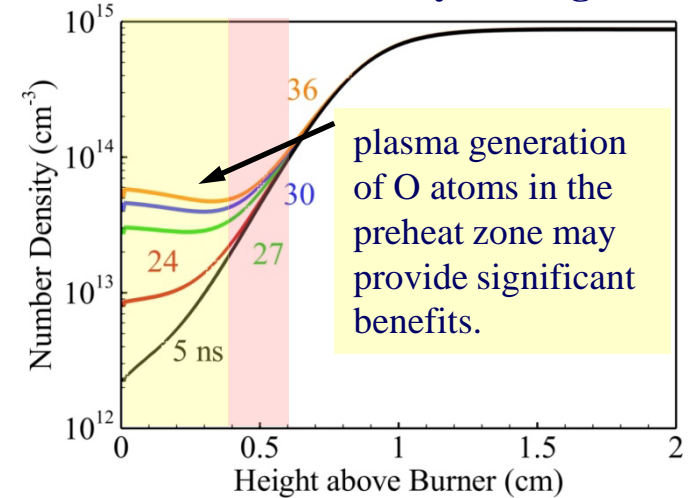
## physical setup



## N<sub>2</sub> excited species vs height



## O atom density vs height



- the production rates of N<sub>2</sub>(A<sub>3</sub>) and N<sub>2</sub>(B<sub>3</sub>) in the preheat zone is about 2 times higher than downstream because of higher N<sub>2</sub> number density.
- electron impact dissociation of O<sub>2</sub> in the preheat zone results in ~30 times increase in O atom density within 30 ns
- the excited species are quenched rapidly after the pulse resulting in further production of O and other radicals

## ongoing work

- we are performing longer timescale simulations to understand the effect of repetitive application of discharge pulses on flame dynamics.
- the effect of NS discharges on H<sub>2</sub>-air, CH<sub>4</sub>-air and C<sub>2</sub>H<sub>4</sub>-air premixed flames are being investigated.
- close collaboration with OSU group is pursued for obtaining greater insight through experiments and high fidelity modeling

## **High fidelity 1D numerical tools for construction and validation of robust plasma combustion kinetic models**

- detailed studies of the plasma coupled premixed flame system for a variety of fuels.
- development of the counterflow plasma flame simulation framework.
- close collaboration with other MURI team members for model validation and critical assessment of the plasma combustion kinetic models

## **2D/3D simulations of nonequilibrium plasma in complex flow environments**

- High fidelity simulations of single filament discharge in 2D with detailed chemistry.
- Large Eddy Simulation (LES) of  $H_2$  jet in supersonic  $O_2$  crossflow in the presence of a nanosecond plasma source.
- theoretical framework to understand plasma-flow interactions.